

Observations of the O(³P) fine structure line at 63 μm in the upper mesosphere and lower thermosphere

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[1] Observations of the O(³P) fine structure line at 63 μm originating in the upper mesosphere and lower thermosphere have been obtained by the far-infrared spectrometer (FIRS-2) instrument, a Fourier transform spectrometer that flies periodically on high-altitude balloons. FIRS-2 primarily observes stratospheric ozone photochemistry using the technique of limb emission spectroscopy. As part of the routine operation of FIRS-2, up-looking views are made, during which the emission from the atomic oxygen is recorded. Using the Mass Spectrometer Incoherent Scatter (MSIS) empirical model to provide temperature and atomic oxygen concentrations, we compute radiances for comparison with the FIRS-2 observations. The computed radiances agree with the FIRS-2 measurements, which encompass 31 observations during nine flights over a span of 14 years, to within 10% on average, with 23 of the 31 observations agreeing to within measurement and calculation uncertainty. The consistency between the observed and computed radiances suggests that the MSIS model provides a reasonably accurate representation of temperature and atomic oxygen in the upper mesosphere and lower thermosphere. **INDEX TERMS:** 0355 Atmospheric Composition and Structure: Thermosphere—composition and chemistry; 0340 Atmospheric Composition and Structure: Middle atmosphere—composition and chemistry; 0358 Atmospheric Composition and Structure: Thermosphere—energy deposition; 3359 Meteorology and Atmospheric Dynamics: Radiative processes; **KEYWORDS:** atomic oxygen, far-infrared, oxygen emissions, thermospheric energy balance

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1. Introduction

[2] Infrared radiative cooling of the upper mesosphere and lower thermosphere is dominated by emission from three species: carbon dioxide at 15 μm [Curtis and Goody, 1956], nitric oxide at 5.3 μm [Kockarts, 1980], and atomic oxygen at 63 μm [Bates, 1951]. Of these three the emission from atomic oxygen is the least observed, owing in part to the challenge of measuring radiation at far-infrared wavelengths. The emission is unobservable from ground-based instruments because of the complete absorption by tropospheric water vapor. At present the 15- μm CO₂ emissions and the 5.3- μm NO emissions are being observed globally by the Thermosphere-Ionosphere-Mesosphere Energetics

and Dynamics (TIMED) satellite, which was launched in 2001. The goal of TIMED is to quantify the energy budget of the upper mesosphere and lower thermosphere [e.g., Mlynczak, 1995, 1997]. In contrast, the atomic oxygen emission has been observed in a handful of rocket flights [Grossman and Vollmann, 1997] and most extensively by the CRISTA payload that flew on the space shuttle in the 1990s [Grossman *et al.*, 2000]. Analysis of the CRISTA data was restricted to altitudes above 130 km because of the opacity of this transition in the limb view employed by CRISTA.

[3] In this paper we report a series of observations of the atomic oxygen emission at 63 μm made by an instrument operating periodically on a high-altitude (~38-km) balloon payload. The observations are compared against radiative transfer calculations that use temperature and atomic oxygen from the Mass Spectrometer Incoherent Scatter (MSIS) empirical model [Hedin, 1991]. There are 31 extant observations from nine separate flights during spring, summer, and fall over a span of 14 years. Agreement between the radiative transfer calculations and the observed radiances is better than 10% for 21 of the 31 observations, and four of the remaining 10 agree to within 15%. The far-infrared spectrometer (FIRS-2) observations are described in

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Table 1. The 31 Radiance Observations of the O(³P) Fine Structure Line (FIRS-2), Estimated Uncertainty (Error Percent), and Comparison With Radiative Transfer Calculations (MSIS)^a

Observation	Date	Time, UT	FIRS-2	Error, %	MSIS
1	26 Sept. 1989	2249:43	1.962	7.1	2.315
2	27 Sept. 1989	0350:54	2.535	5.1	2.281
3	05 June 1990	0734:51	2.165	3.5	1.880
4	05 June 1990	1624:51	1.932	4.6	1.932
5	05 June 1990	1846:19	2.228	5.0	2.053
6	29 May 1992	1705:10	1.884	8.8	1.917
7	29 May 1992	2010:41	1.917	5.2	1.947
8	29 Sept. 1992	1748:43	2.214	7.8	2.208
9	29 Sept. 1992	2034:27	1.969	6.9	2.196
10	29 Sept. 1992	2240:13	1.954	9.8	2.067
11	24 March 1993	0312:13	2.051	7.9	2.024
12	24 March 1993	0456:28	2.295	10.2	2.109
13	24 March 1993	0707:28	2.154	7.0	2.112
14	22 May 1994	1813:57	2.006	5.8	1.824
15	22 May 1994	2212:49	1.917	6.7	1.710
16	22 May 1994	2439:13	1.888	6.1	1.615
17	23 May 1994	0531:10	1.806	5.2	1.773
18	23 May 1994	0849:28	2.021	6.3	1.670
19	23 May 1994	1332:51	1.510	8.0	1.609
20	30 April 1997 ^b	1836:59	1.695	5.2	1.518
21	30 April 1997 ^b	2053:05	1.839	5.2	1.574
22	30 April 1997 ^b	2242:47	1.684	4.8	1.606
23	20 Oct. 2002	1907:48	2.510	7.3	2.371
24	19 Sept. 2003	1736:36	2.040	6.3	2.140
25	19 Sept. 2003	1958:48	2.010	6.8	2.162
26	19 Sept. 2003	2146:12	1.700	8.7	2.070
27	19 Sept. 2003	2332:24	1.830	8.2	1.969
28	20 Sept. 2003	0237:48	2.050	6.8	2.015
29	20 Sept. 2003	0444:24	2.070	5.4	2.105
30	20 Sept. 2003	0707:12	1.970	5.4	2.077
31	20 Sept. 2003	0924:24	1.880	4.9	2.000

^aFormats are as follows: date, day/month/year; universal time, hour/minute/second; radiances, nW cm⁻² sr⁻¹. Observations are at 35°N, 104°W.

^bObservations are at 66°N, 150°W.

section 2, followed by a discussion of the radiative transfer modeling in section 3. The paper concludes with a discussion and summary in section 4.

2. Description of the 63-μm Observations

[4] The atomic oxygen emission at 63 μm is observed by the Smithsonian Astrophysical Observatory FIRS-2 instrument, which is a Fourier transform spectrometer that measures the thermal emission of the terrestrial atmosphere from balloon and aircraft platforms and from the ground. FIRS-2 routinely observes ozone, water vapor, hydroxyl, and other minor species relevant to stratospheric ozone photochemistry. The instrument covers the far-infrared portion of the spectrum from 80 to 700 cm⁻¹ (extended to 1250 cm⁻¹ in 1997) at an unapodized resolution of 0.004 cm⁻¹. Liquid helium cooled photoconductor detectors are used, with a gallium-doped germanium detector covering 80–320 cm⁻¹ and a copper-doped germanium detector covering 320–1250 cm⁻¹. The instrument and data reduction system are described by *Johnson et al.* [1995].

[5] The data presented here were obtained during nine balloon flights launched between 1989 and 2003. The dates and times of each flight and O(³P) radiance observation are listed in Table 1. With the exception of the 1997 flight,

which took place at 66°N latitude, all flights were launched near 35°N latitude at Fort Sumner, New Mexico. The FIRS-2 spectra are calibrated in intensity using an onboard blackbody source (typically operating near 0°C) and a space view at an elevation angle of 30° above the horizon, i.e., 60° down from zenith. The spectra obtained during the space view from a typical balloon altitude of 38 km contain a few narrow emission lines. The O(³P) fine structure line is an unmistakable feature of the space look spectrum. Shown in Figure 1 is an example of the atomic oxygen emission line as recorded by FIRS-2 during a flight in May 1994. Listed in Table 1 are the spectrally integrated radiances (nW cm⁻² sr⁻¹) measured by FIRS-2 in 31 separate observations made over the course of the nine flights. The radiances are typically obtained from an average of four to six spectra each, requiring between 11 and 16 min of integration time to record. The maximum observed radiance from the 1989 flight is ~65% larger than the minimum observed value from the flight in 1994. The total estimated uncertainty of each measurement is listed in Table 1. The error analysis of these measurements is discussed in section 4. The 63-μm line was also observed by the FIRS-1, the predecessor to the FIRS-2 instrument, in a flight in June 1982. The O(³P) observations from that flight were reported by *Lin et al.* [1987], who gave a radiance value of 1.7 (±0.2) nW cm⁻² sr⁻¹. As indicated in the results listed in Table 1, the Lin et al. measurement falls within the range of approximately one half of the FIRS-2 measurements when the uncertainties of each instrument are taken into account.

3. Radiative Transfer Calculations

[6] We compare the FIRS-2 measurements of the spectrally integrated radiance from O(³P) at 63 μm with radiative transfer calculations using the MSIS-90 atmospheric model to provide vertical profiles of atmospheric temperature and atomic oxygen as inputs into the radiative transfer model. MSIS is an empirical model that is based on observations from mass spectrometer instruments that flew on a series of orbiting satellites and also on the space shuttle in addition to observations from ground-based incoherent scatter radars. The atmospheric variability is computed in the model based on the $F_{10.7}$ solar flux index and the A_p magnetic index. The MSIS model is described by *Hedin* [1991].

[7] We simulate the radiance emitted by the atmosphere by evaluating the radiative transfer equation using the MSIS profiles as inputs. The radiative transfer equation that we evaluate is

$$R = \int_v \int_z B_v(T(z)) \frac{\partial \tau_v}{\partial z} dz dv, \quad (1)$$

where R is the spectrally integrated radiance (nW cm⁻² sr⁻¹) and $B_v(T(z))$ is source function evaluated at altitude z at temperature T . As will be shown later in this section, the bulk of the radiance observed by FIRS-2 originates below ~140-km altitude, so that local thermodynamic equilibrium (LTE) can be assumed for the transition [*Sharma et al.*, 1994]. Under LTE the source function B_v is identical to the Planck blackbody function. The term $\partial \tau_v / \partial z$ is the derivative of the monochromatic atmospheric transmittance

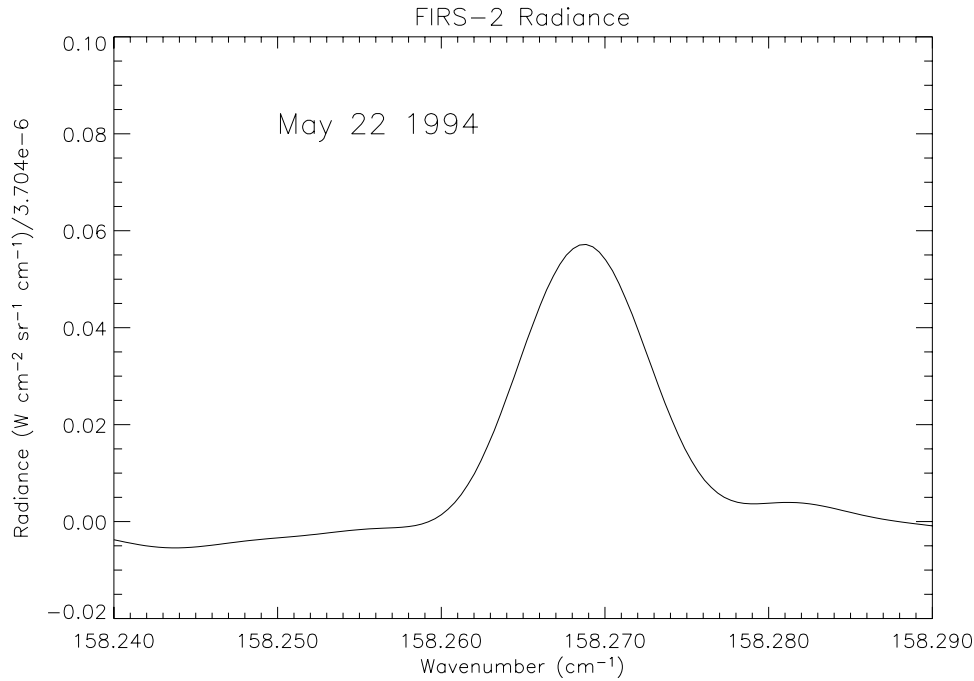


Figure 1. Observed FIRS-2 spectrum of the atomic oxygen fine structure line at 63 μm on 22 May 1994.

τ_ν . The integral is over wave number ν and over altitude z . The monochromatic transmittance τ_ν is defined by

$$\tau_\nu = \exp(-k_\nu u), \quad (2)$$

where k_ν is the absorption cross section and u is the optical mass, both calculated along the line of sight. The absorption cross section is defined as the product of the line strength S and the line shape function, which is taken to be the Doppler function. The line strength S is obtained from the HITRAN 2000 database [Rothman *et al.*, 2003]. At 296 K the line strength is $1.131 \times 10^{-21} \text{ cm}^{-1}/(\text{atom cm}^{-2})$, which corresponds to an inverse radiative lifetime of $8.797 \times 10^{-5} \text{ s}^{-1}$, or a radiative lifetime of ~ 3.1 hours. Despite the long radiative lifetime, which would generally imply a weak transition, the radiative transfer for the fine structure line is not in the optically thin limit of radiative transfer in the upper mesosphere and lower thermosphere owing to the very narrow Doppler broadened line and the large atomic oxygen abundances. In the radiation transfer calculations the line strength S is corrected for temperature according to the standard relationship

$$S(T) = S(T_{\text{ref}}) \frac{Q(T_{\text{ref}})}{Q(T)} \frac{\exp(-E_L/kT)}{\exp(-E_L/kT_{\text{ref}})} \frac{1 - \exp(-h\nu/kT)}{1 - \exp(-h\nu/kT_{\text{ref}})}, \quad (3)$$

where Q is the electronic partition function, E_L is the energy above ground of the lower state of the transition, ν is the frequency in cm^{-1} , and T_{ref} is the reference temperature at which the line strength is given on the HITRAN database, 296 K. The last term in equation (3) is the correction for stimulated emission. We note that E_L is zero for the 63- μm line but that the electronic partition function and the

stimulated emission terms are significantly different from unity.

[8] We compute the atmospheric radiance that would be sensed by FIRS-2 with three independently developed radiative transfer codes. The radiance is calculated using the Full Transfer by Ordinary Line-by-Line Methods (FUTBOLIN) radiative transfer code [Martin-Torres *et al.*, 2003] and the Monochromatic Radiative Transfer Algorithm (MRTA) code [Kratz *et al.*, 1998]. Both the FUTBOLIN and MRTA codes have recently participated in a radiation code comparison exercise, with extremely favorable comparisons with several other codes in the far-infrared portion of the spectrum [Kratz *et al.*, 2005]. Last, a third radiative transfer code was specifically written for the computation of the radiance from the O(³P) 63- μm line.

[9] Each of these three codes evaluates the monochromatic radiance across the 63- μm line at high ($\leq 0.00004 \text{ cm}^{-1}$) spectral resolution, typically one-fifth the smallest Doppler half width, thus assuring proper sampling of the spectral line shape. The monochromatic radiances are then integrated to obtain the radiance in units of $\text{nW cm}^{-2} \text{ sr}^{-1}$ for comparison with the FIRS-2 observations. The integration is carried out more than five Doppler half widths from line center in order to capture all of the radiation emitted by the line. Radiances computed by the three codes agreed among themselves to better than 1% for all 31 MSIS atmospheres corresponding to the FIRS-2 observations.

[10] The atmosphere profiles provided by MSIS and used in the radiative transfer calculations extend from 75 to 400 km at a spacing of 1 km. The MSIS values of temperature and atomic oxygen are used to define the source function, the cross sections, the optical mass, and the monochromatic transmittances within each 1-km layer. The monochromatic transmittance from 75 to 400 km is

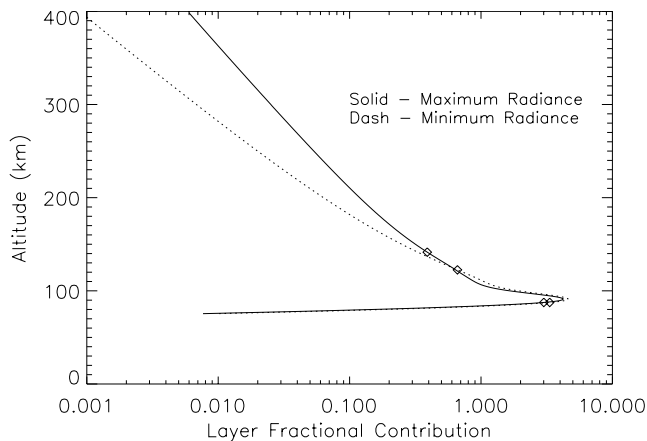


Figure 2. Fractional contributions from each 1-km atmospheric layer to the total radiance as observed by FIRS-2 on the basis of MSIS simulations of the observation at 0350:04 on 27 September 1989 (solid curve) and of the observation at 1332:51 on 23 May 1994 (dashed curve). Results indicate the peak contribution to the radiance is from the layer at 92 km. Diamonds indicate the altitudes on each curve below which 10 and 80% of the total observed radiance occurs.

computed, and the transmittance gradient is then evaluated for each 1-km layer and multiplied by the source function for that layer, yielding the radiance emitted by that layer that would arrive at the FIRS-2 instrument. A plane-parallel atmosphere is assumed, and the path length is computed using a 60° zenith angle.

[11] To determine the atmospheric regions from which the 63- μ m radiation arises, we have computed the ratio of the radiance emitted by each 1-km layer to the total radiance emitted by the atmosphere along the line of sight to FIRS-2. Shown in Figure 2 is a plot of this ratio for the two MSIS atmosphere profiles corresponding to conditions of the FIRS-2 maximum (solid curve) and minimum (dashed curve) radiance measurements. The results in Figure 2 indicate that the atmospheric layer near 92 km contributes the maximum radiance to the FIRS-2 observations, an altitude that is approximately 4–6 km below the altitude at which the peak atomic oxygen concentration typically occurs in the MSIS model. However, the results in Figure 2 also indicate that the atmospheric emission sensed by FIRS-2 arises over a broad altitude span. The altitudes below which 10 and 80% of the simulated radiances arise are indicated by diamonds on the curves in Figure 2. Ten percent of the radiance originates below \sim 87 km, and 80% originates below \sim 125–140 km. The contributions from the thermosphere are due to the increasing temperature with altitude in the thermosphere that results in both a larger source function and a broader spectral line, the latter of which emits radiation at frequencies that are not absorbed in the cooler lower atmosphere and hence are sensed by FIRS-2. Note that the dashed curve with a smaller contribution in the midthermosphere corresponds to a cooler thermosphere with less atomic oxygen. Although these results are for model calculations, we believe they closely represent the atmospheric contributions.

[12] The cumulative contribution to the total radiance as a function of altitude is obtained by integrating the radiance

contributions from each layer (i.e., those in Figure 2). The result of this integration is shown in Figure 3. We again show two curves, corresponding to the maximum (solid curve) and the minimum (dashed curve) radiance conditions sensed by FIRS-2. Although the bulk of the radiance originates below 140 km, more than 5% of the radiance observed under the maximum radiance conditions originates above 200 km. To begin to assess the agreement between the measurements and the models, we show in Figure 4 a plot of the measured FIRS-2 radiances and the radiances computed using the MSIS atmospheres. This plot is indicative of the agreement between the measured and modeled radiances. The data possess a linear correlation coefficient of 0.675. The computed radiances agree to within 10% of the measured radiances in 21 of 31 observations and to within 15% in four of the remaining ten observations.

4. Discussion

[13] The agreement shown in Figure 4 between the measured and modeled radiances and the contribution functions shown in Figures 2 and 3 illustrate the unique nature of the FIRS-2 observations. The bulk of the radiation observed by FIRS-2 originates in the lower thermosphere and upper mesosphere (80–140 km). In contrast, the space-based observations from the CRISTA instrument on the space shuttle [Grossman *et al.*, 2000] are limited to the altitude range from 130 to 170 km because of the atmospheric opacity. Thus the FIRS-2 observations represent an opportunity to evaluate the consistency of MSIS temperature and atomic oxygen profiles in an altitude region that is not accessible by space observation. We note that the CRISTA team used temperatures from MSIS to retrieve atomic oxygen and obtained results that were 40% smaller than the corresponding MSIS atomic oxygen values.

[14] In order to assess the measured and computed 63- μ m radiances we must first consider the uncertainty associated with the measurement and with the computations. We consider first the systematic uncertainty and precision of the radiance measurements. The systematic uncertainty is

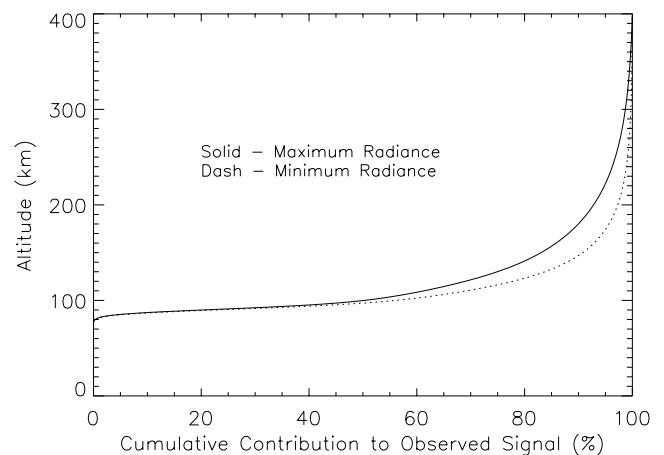


Figure 3. Cumulative contribution to the total radiance as observed by FIRS-2 on the basis of the same MSIS simulations in Figure 2. In both cases, over 80% of the total radiance arises from altitudes below 140 km.

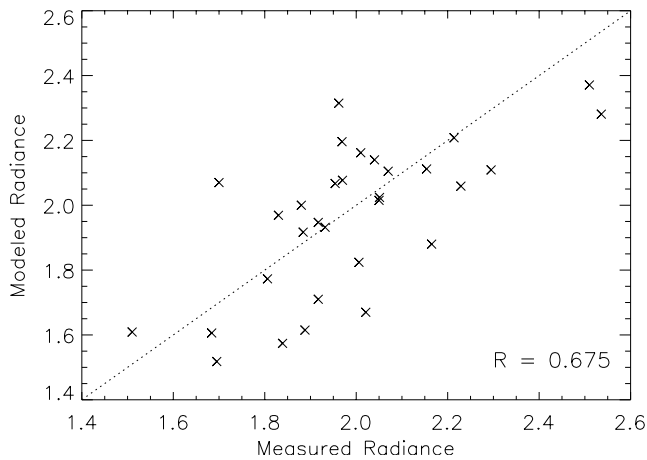


Figure 4. FIRS-2 measured radiance plotted versus the MSIS modeled radiance. Units are $\text{nW cm}^{-2} \text{sr}^{-1}$. Linear correlation coefficient R for the data is 0.675.

estimated to be 2% for each of the radiance measurements, while the precision of the measurement is different for each observation and dependent on FIRS-2 instrument and flight conditions. The estimated precisions are between 4 and 10%, depending on flight. To obtain the total uncertainty for each measurement, we calculate the root-sum-square of the systematic uncertainty and the precision. The resulting uncertainties range from 4.5 to 10.2%, with a mean of 6.5%, and are listed individually for each flight in Table 1.

[15] Uncertainties in the radiance calculations may arise from several sources, including the atmospheric temperature, the atomic oxygen concentration, and the transition line strength. We assess the potential uncertainties in each of these by varying each one in turn and computing the associated change in the radiance. A change in the line strength of 5% corresponds to a change in the radiance of 1.5%. Varying the atomic oxygen profile at all altitudes by 10, 20, and 30% (with temperature held constant) changes the calculated radiance on average by 3.5, 7, and 10%, respectively. Varying the temperature profile by 10 K at all altitudes (with atomic oxygen held constant) changes the calculated radiance by 6.9% on average.

[16] Shown in Figure 5 is a plot of the FIRS-2 measurements (crosses) with error bars corresponding to the estimated uncertainty of each measurement. Also shown are the computed radiances (triangles) with error bars corresponding to the root-sum-square of the uncertainties due to a 5% uncertainty in line strength, a 5 K uncertainty in temperature, and a 10% uncertainty in atomic oxygen, for an overall uncertainty of 5% in the calculated radiances. The error bars overlap in 23 of the 31 cases, with two additional cases nearly overlapped. Thus MSIS temperatures and atomic oxygen faithfully reproduce the FIRS-2 observations over a large span of geophysical conditions including the solar cycle, the annual and seasonal cycles, and daily local time variability. We therefore conclude that the MSIS temperatures and atomic oxygen profiles in the upper mesosphere and lower thermosphere are consistent with the FIRS-2 observations. This result is in contrast to that derived in the middle thermosphere from the CRISTA measurements.

[17] The measurements shown in Figure 5 indicate a smaller magnitude of the $63\text{-}\mu\text{m}$ emission in observations 14–22 which were made during two flights in 1994 and 1997. These lower values are obtained during the declining phase of the solar cycle. We note that the calculated MSIS radiances are also smaller during this time. These results are suggestive of a solar cycle dependence in the radiances, as reduced solar activity should lead to a cooler lower thermosphere with lower atomic oxygen and hence lower $63\text{-}\mu\text{m}$ emission. Because the MSIS model results depend on the $F_{10.7}$ solar flux, we computed the linear correlation coefficient between the observed daily and 3-month average $F_{10.7}$ flux and the FIRS-2 radiances, obtaining values of 0.725 and 0.597, respectively. These results suggest a correlation with solar variability dependent more on the immediate solar conditions than on built-up longer-term effects. Shown in Figure 6 is a plot of the $63\text{-}\mu\text{m}$ radiances computed hourly over the course of a day (22 May 1994) using temperature and atomic oxygen from MSIS. The variability is predicted to have a semidiurnal component. We conclude that the variability in the $63\text{-}\mu\text{m}$ emission as observed by FIRS-2 is likely influenced by diurnal and semidiurnal effects and also by the longer-term variability of the Sun. The FIRS-2 data, while suggestive of solar cycle dependence, are too sparse to allow any definitive geophysical effect to be attributed to the observed variation.

[18] We can, however, determine specifically the reasons for the observed changes in radiance. There are two parameters in the radiative transfer equation, the source (Planck) function and the transmittance gradient. The source function depends solely on temperature under the assumed conditions of local thermodynamic equilibrium. The transmittance gradient depends on the atomic oxygen abundance and to a lesser extent on temperature through the absorption cross section. In the far-infrared the Planck function is a relatively weak function of temperature. For the range of

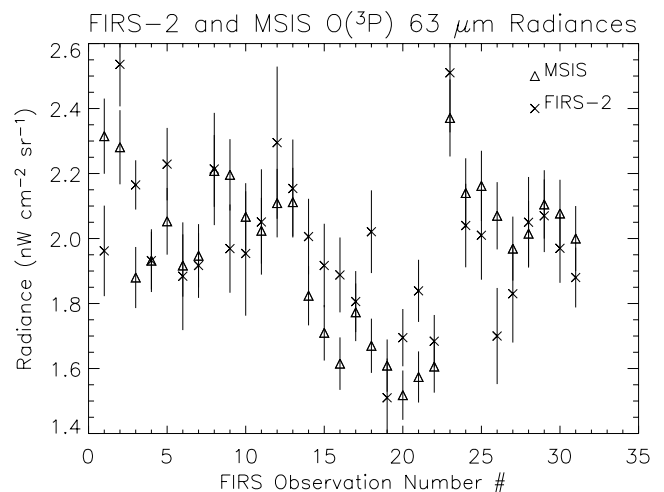


Figure 5. FIRS-2 observed radiances (crosses) with error bars representing measurement accuracy plotted with MSIS-calculated radiances (triangles) with error bars representing calculation uncertainty of 5%, as described in the text. Error bars overlap in 23 of the 31 cases. Measurements are arranged in time sequence order corresponding to the list in Table 1.

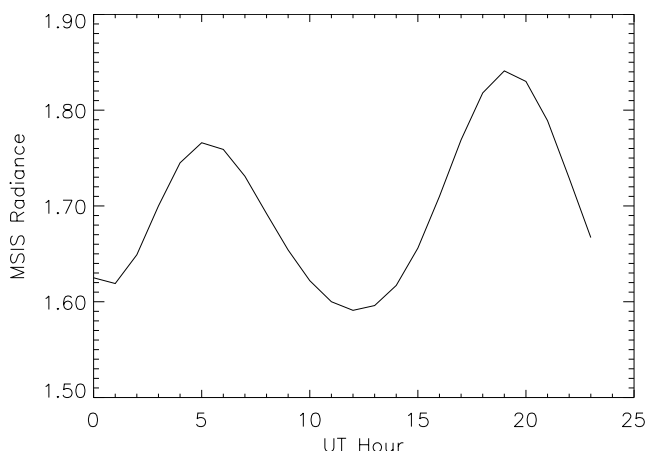


Figure 6. Hourly time series of O(³P) 63- μ m radiance ($\text{nW cm}^{-2} \text{sr}^{-1}$) as would be observed by FIRS-2 computed with the MSIS model atmosphere on 22 May 1994. Calculations indicate a semidiurnal variability in far-infrared radiance.

temperatures predicted by the model for the observed maximum and minimum radiance conditions, the Planck function changes by no more than 10% below 200 km. In contrast, the MSIS atomic oxygen changes by 30% to 70% over the altitude range from 90 to 140 km over these conditions. This result indicates that changes in atomic oxygen are predicted to be mostly responsible for the observed changes in 63- μ m radiance. In Figure 7 we plot the computed MSIS radiance for the FIRS-2 observation times against the MSIS column atomic oxygen between 80 and 150 km. The linear correlation coefficient for these data is 0.91. We conclude that the model radiances are driven by variations in atomic oxygen. In Figure 8 we show the FIRS-2 radiances plotted against the model column atomic oxygen. The linear correlation coefficient is 0.649. We conclude that the observed radiance variation is likely due

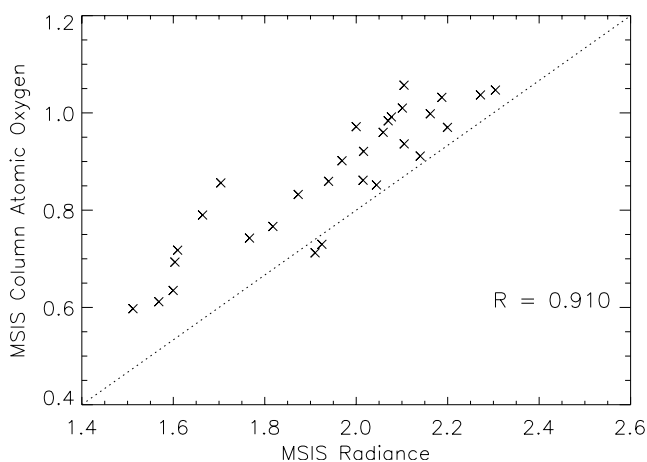


Figure 7. MSIS 63- μ m radiance ($\text{nW cm}^{-2} \text{sr}^{-1}$) for the FIRS-2 observation times plotted against MSIS column atomic oxygen. Linear correlation coefficient R is 0.910. Results imply that the major cause of changes in radiances computed with the MSIS atmosphere is changing atomic oxygen abundances.

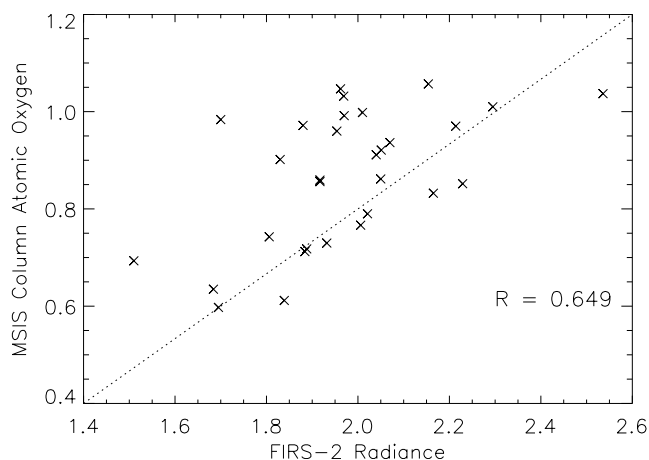


Figure 8. FIRS-2 radiances ($\text{nW cm}^{-2} \text{sr}^{-1}$) plotted against the corresponding MSIS column atomic oxygen. Linear correlation coefficient R is 0.649.

to a combination of atomic oxygen and temperature variability, with atomic oxygen variability likely being the dominant cause of the radiance variation and temperature variability potentially being more of a factor than predicted by the model.

5. Summary

[19] We have presented 31 measurements of radiance emitted by the thermospheric fine structure line of atomic oxygen at 63 μm observed from a high-altitude balloon payload during nine separate flights over a period of 14 years. The observed radiation originates in the upper mesosphere and lower thermosphere below 140 km. The measured radiances vary by $\sim 65\%$ over the time period. Radiative transfer calculations using MSIS empirical model temperatures and atomic oxygen densities agree with the observations to generally better than 10%, which is remarkable given the span of time and geophysical conditions over which the observations are made. Twenty-three of the 31 comparisons agree to within the uncertainties of the measurements and calculations. Although discrepancies between MSIS temperature and atmospheric observations have been noted [e.g., *Sharma and Duff, 1997*], and although MSIS could not be expected to replicate the thermal structure during strongly perturbed events such as the dramatic solar storms of 2002 [e.g., *Mlynchak et al., 2003*], the consistency between the measured radiances and the computed radiances suggests that the MSIS model is a reasonably accurate representation of the temperature and atomic oxygen concentrations in the upper mesosphere and lower thermosphere under a wide range of conditions.

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